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High performance explosive molecules

Laurence E. Fried, Christine Wu, Glenn Fox, and Philip Pagoria

In this project we are seeking to substantially accelerate the development of new high performance explosive molecules. By combining state of the art quantum chemistry calculations with the aggressive synthetic pursuit of promising candidate molecules, we hope to advance the state of the art in this field more than 50 years.

There are several drivers for new high performance explosives in the DoD. The transition from bulk fill bombs to small smart weapons system puts a premium on performance upon delivery and high energy density. Higher performance materials could also be important in future DOE explosive-driven experiments.

Our approach is based on the tight linkage of theory with chemical synthesis. We have established a high explosive performance prediction code by linking the thermochemical code CHEETAH with the ab initio electronic structure code GAUSSIAN and the molecular packing code MOLPAK.

GAUSSIAN is first used to determine the shape of the molecule and its binding energy. The molecules are then packed together into a low energy configuration by MOLPAK. Finally CHEETAH is used to transform the crystal energy and density into explosive performance measures such as detonation velocity, pressure, and energy.

We have benchmarked our performance prediction system against a large number of known explosives of varying performance. In Figure 1 we compare performance with calculated crystal properties to performance with actual crystal properties.

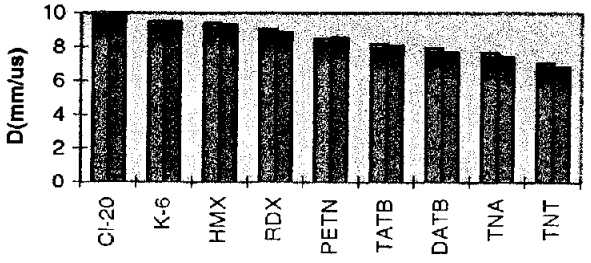

Figure 1: Detonation velocities based on experimental HE energy and density (maroon) compared to theoretical detonation velocities (blue).

The theoretical chemists (Fried,Wu) and the organic chemists (Pagoria, Fox) involved in this project have worked together to create over 70 target molecules. Performance calculations were then undertaken for each of the possible targets.

Of the many target molecules, several showed great promise in combining performance, chemical stability, and ease of synthesis. We are now pursuing the synthesis of these final target molecules.

In Figure 2, we show one of our the target molecules, which is currently being synthesized by Glenn Fox. This molecule uses a combination of multiple chemical bonds and bicyclic ring structure to achieve high predicted density (2.15 g/cc) and energy (1.4 times HMX, the material with the highest energy in common use today). If successful, the synthesis of this material will produce the most powerful explosive known today.

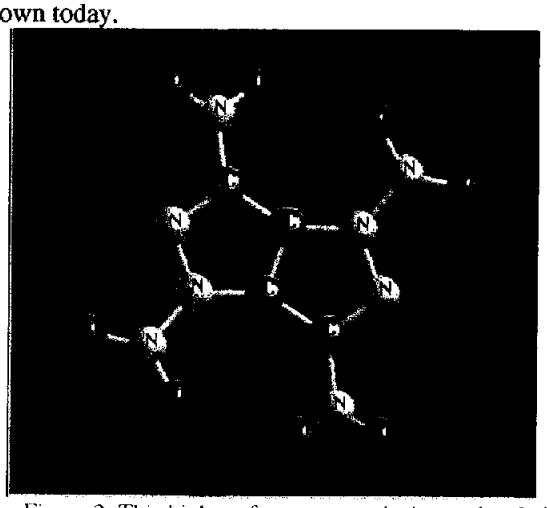

Figure 2: This high performance explosive molecule is currently being synthesized. Its predicted performance is 1.4 times HMX.

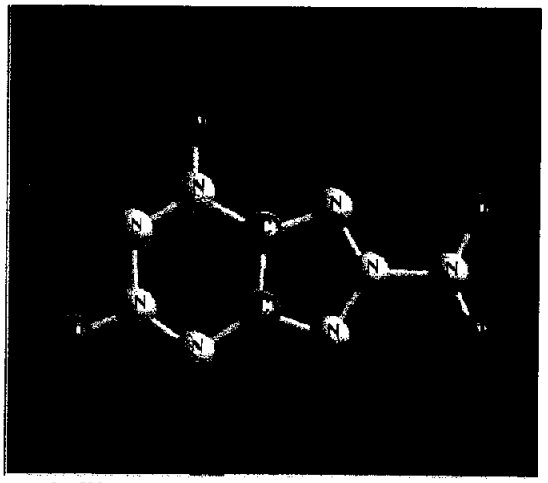

Figure 3: We are beginning synthesis of this super-HE (1.8 times HMX).

We are also pursuing more difficult target molecules. We show one of our forefront materials (1.8 x HMX) in Figure 3. This molecule could revolutionize the use of explosives in critical applications

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